

Supplementary Information

Title: Synthetic and Structural Studies on New Diiron Azadithiolate (ADT)-Type Model Compounds for Active Site of [FeFe]Hydrogenases

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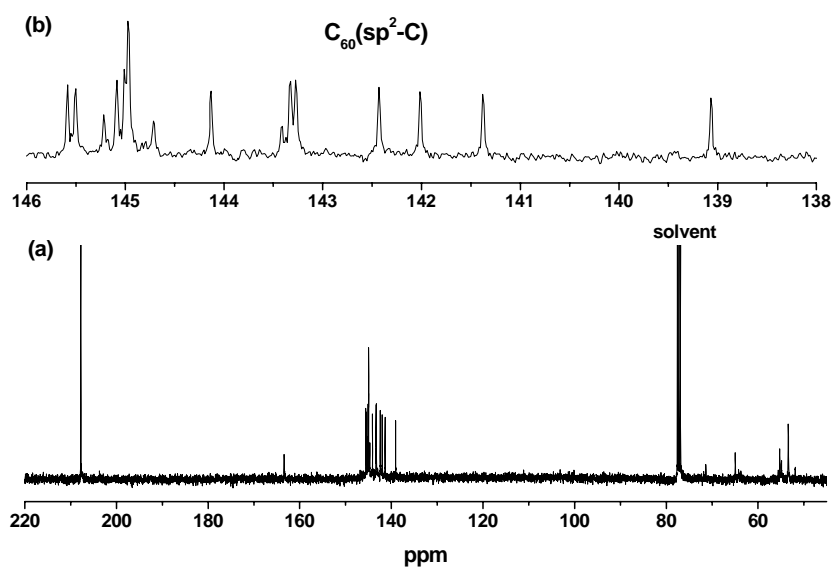


Fig. S1a (a) Original ^{13}C NMR spectrum of **7**. (b) Expanded ^{13}C NMR spectrum of **7**.

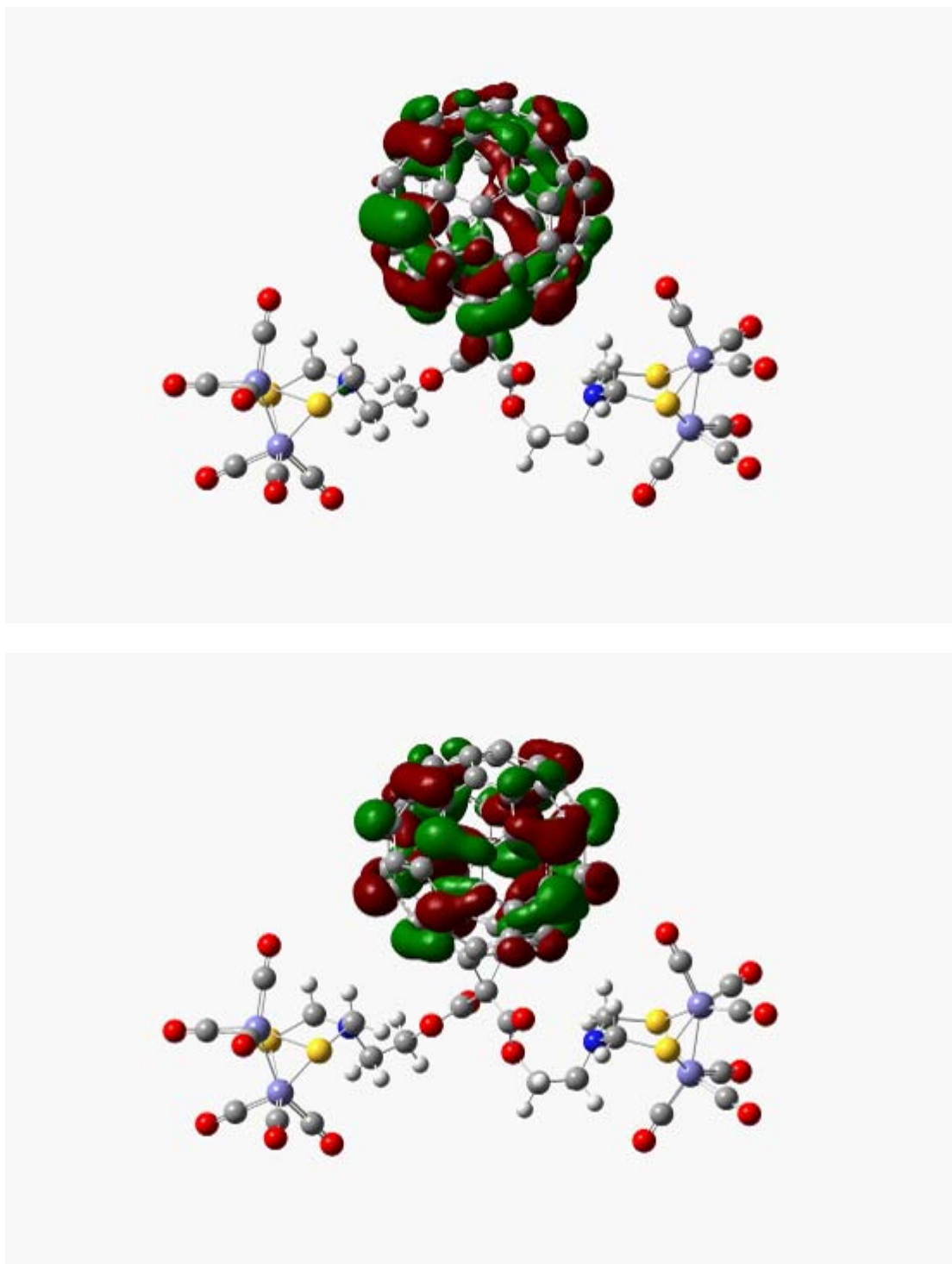


Fig. S1b Frontier orbitals of **7** : HOMO(top) and LUMO (bottom).

Table S1 Comparisons between the experimental and computational IR frequencies and intensities of **6–8**.

	vib. mode	Experimental		Computational	
		freq. (cm ⁻¹)	int.	freq. (cm ⁻¹) ^a	int.
6	$\nu_{\text{C=O}}$	1746	s	1754,1768	168, 26
	$\nu_{\text{C}\equiv\text{O}}$	1993	vs	1998,2007, 2007	203, 645, 299
	$\nu_{\text{C}\equiv\text{O}}$	2031	vs	2024, 2028	1068, 1872
	$\nu_{\text{C}\equiv\text{O}}$	2071	s	2074	760
7	$\nu_{\text{C=O}}$	1748	s	1756, 1769	138, 107
	$\nu_{\text{C}\equiv\text{O}}$	1993	vs	1997,1998,2006, 2008, 2008	143, 236, 1229, 116, 465
	$\nu_{\text{C}\equiv\text{O}}$	2031	vs	2024,2025,2027, 2028	806, 1307, 475, 3073
	$\nu_{\text{C}\equiv\text{O}}$	2072	s	2074, 2075	1272, 304
8	$\nu_{\text{C=O}}$	1746	s	1754, 1764	152, 55
	$\nu_{\text{C}\equiv\text{O}}$	1932	s	1972, 1985	181, 120
	$\nu_{\text{C}\equiv\text{O}}$	1981	vs	1997, 2007	1881, 781
	$\nu_{\text{C}\equiv\text{O}}$	2042	vs	2049	1141

^aThe computed frequencies are scaled by 0.9631 as suggested for the B3LYP/6-31G(d) level of theory.¹

1. J. B. Foresman and A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian, Inc., Pittsburgh, PA, 1996.

